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A FREQUENTIAL ANALYSIS OF THE NUMERICAL ALGORITHMS USED FOR INVERSE FILTERING IN CALORIMETRY

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ABSTRACT

The performances are evaluated of the inverse filters commonly used to eliminate poles and zeros from the transfer function of the calorimetric system. The analysis is carried out in frequency space, by means of the Z-transform. The algorithms are tested on models covering the full dynamic range attainable for heat conduction calorimeters. As relative scales are used for time and frequency, the results of the analysis can be applied in any experimental device.

INTRODUCTION

A study of the dynamic behaviour of several different calorimetric devices has shown that inverse filtering is a well-suited numerical tool to perform the identification of the system and the deconvolution of the thermograms. For example, inverse filtering has been used to obtain the instantaneous thermal power released during a thermally-induced martensitic transformation or during continuous injection of the solute in a binary liquid mixture [1–4]. The generalization of inverse filtering to deal with deconvolution in time-varying systems has also been studied [5, and references therein].

Generally speaking, inverse filtering is applied in thermograms which are sampled with a sampling period Δt. The choice $\Delta t \approx \tau_1/300$, where τ_1 is the main time constant of the calorimeter, has been proposed [6]. The sampling of the thermogram leads, in the filtering process, to numerical algorithms in which the derivatives of the signal are replaced by finite differences; hence, the correction achieved is progressively different from what would be obtained applying an exact inverse filtering. In principle, the deconvolution could be performed by means of the Z-transform, which explicitly takes into account the discreteness of the thermogram. Unfortunately, the Z-transform presents serious difficulties in dealing with time-varying systems.

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A general analysis, showing to what extent the sampling of the thermogram affects the inverse filtering and giving conditions to choose properly the parameters entering the numerical algorithm has not, to our knowledge, been done before. In this paper, we study the performances of numerical inverse filtering depending on the different parameters that have to be chosen in the calculations and on the signal-to-noise ratio in the thermogram. The investigation covers the whole domain of work—in a relative scale [7]—of heat conduction calorimeters.

NUMERICAL ALGORITHMS

To eliminate the effect of the ith pole in the transfer function of the calorimeter, the appropriate inverse filter reads

$$s'(t) = s(t) + \tau_i \frac{\mathrm{d}s(t)}{\mathrm{d}t} \tag{1}$$

where $s(t)$ represents the thermogram, $s'(t)$ the corrected signal and $-1/\tau_i$ is the ith pole. As the thermogram is actually sampled every Δt, we express the derivatives in terms of finite differences

$$s'(I) = s(I) + \tau_i \frac{s(I+K) - s(I-K)}{2K \cdot \Delta t} \tag{2}$$

Correspondingly, to eliminate the effect of the ith zero in the transfer function of the calorimeter, the inverse of eqn. (1) holds

$$s(t) = s^*(t) + \tau_i^* \frac{\mathrm{d}s^*(t)}{\mathrm{d}t} \tag{3}$$

where now $s(t)$ is again the thermogram, and $s^*(t)$ represents the signal after correction. The value $-1/\tau_i^*$ corresponds to the ith zero. Writing the derivative in terms of left-shifted differences leads to the equivalent numerical filter

$$s(I) = s^*(I) + \tau_i^* \frac{s^*(I) - s^*(I-K)}{K\Delta t} \tag{4}$$

from where a recurrent relation for $s^*(I)$ is obtained directly.

The preceding expressions show that the results of numerical inverse filtering will depend on the values τ_i and τ_i^* and on the values of K. Writing $J = I + K$ in eqn. (2) we get

$$s'(J-K) = s(J-K) + \tau_i \frac{s(J) - s(J-2K)}{2K\Delta t}$$

and applying the Z-transform

$$TZ[s'(J-K)] = TZ[s(J-K)] + \tau_i \frac{TZ[s(J)] - TZ[s(J-2K)]}{2K\Delta t}$$

leads to

$$z^{-K}TZ[s'(J)] = TZ[s(J)]\left\{z^{-K} + \tau_i \frac{1 - z^{-2K}}{2K\Delta t}\right\}$$

Hence, the transfer function for the numerical inverse filter of a single pole reads

$$\frac{TZ[s'(J)]}{TZ[s(J)]} = 1 + \tau_i \frac{z^K - z^{-K}}{2K\Delta t}$$

Following the same steps, the transfer function for the numerical inverse filter of a single zero is

$$\frac{TZ[s^*(I)]}{TZ[s(I)]} = \frac{K\Delta t}{K\Delta t + \tau_i^*(1 - z^{-K})} \tag{6}$$

Converting the Z-transforms into Fourier transforms we obtain the corresponding expressions in the frequency space

$$\frac{s'(\omega)}{s(\omega)} = 1 + j\tau_i \frac{\sin(\omega K \cdot \Delta t)}{K\Delta t} \tag{7}$$

and

$$\frac{s^*(\omega)}{s(\omega)} = \frac{K\Delta t}{k\Delta t + \tau_i^*[1 - \cos(\omega K \cdot \Delta t) + j \sin(\omega K \Delta t)]} \tag{8}$$

where j stands for the imaginary unit.

From eqns. (7) and (8) it is possible to compare the results obtained from an exact filtering (the limiting values of the expressions above when $(K\Delta t) \to 0$) with those given by the numerical filters actually used.

RESULTS

The effects of the numerical algorithms have been analysed on three different calorimetric models [8] which cover, in what concerns dynamic properties, the whole spectrum of heat-conduction calorimeters. Models M8 and M9 have transfer functions which correspond to the two extreme dynamic behaviours, while model MI corresponds to an intermediate situation. The parameters (poles and zeros) defining these models are given in Table 1.

Generally speaking, not all the parameters in the transfer function of an actual calorimetric device play an equally significant role. The noise in the thermograms results in a cut-off of the transfer function at high frequencies. In this sense, depending on the signal-to-noise ratio encountered in the thermograms, only partial models are required for a description of the calorimetric dynamics. The partial models that we have chosen (Table 2) are

TABLE 1

Values for τ_i and τ_i^* defining the models M8, M9 and MI

	τ_1									τ_i^*	
M8	192	49	18	–	4	2	1.2	0.4	0.3	–	–
MI	192	49	18	9	–	–	–	–	–	64	–
M9	192	49	–	9	4	–	1.2	0.4	0.3	64	6

TABLE 2

Number of poles (p) and zeros (z), adequate to represent the models M8 and M9 depending on the different signal-to-noise ratios

s/n	40 dB	60 dB	80 dB
M8	$3p$	$3p$	$4p$
M9	$4p, 2z$	$5p, 2z$	$6p, 2z$

represented in Fig. 1A. In a non-rigorous way, it can be considered that for a signal-to-noise ratio $s/n \approx 10^L$ we have $L \approx N - M$, where N is the number of poles and M the number of zeros that can be filtered.

The effect of K (the step in the finite-differences algorithm) has been studied from the divergences between the exact and the discrete filters. The divergences are given by the difference (in dB) between the modulus of the two transfer functions at the frequency under study. Table 3 gives the values of K that should be used when filtering a pole, to keep this difference in the

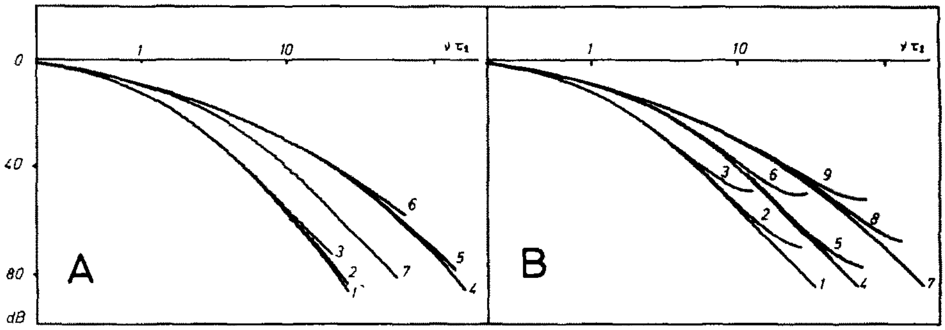

Fig. 1. Moduli in dB, vs. a relative frequency scale, of the transfer functions corresponding to the filters given by the models M8, M9 and MI. (A) Model M8: (1) complete, (2) three poles, (3) four poles. Model M9: (4) complete, (5) four poles and two zeros, (6) five poles and two zeros. Model MI: (7) complete. (B) Model M8: (1) with three poles, (2) numerical approach using $K = 6$, (3) numerical approach using $K = 14$. Model MI: (4) complete, (5) numerical approach using $K = 2$, (6) numerical approach using $K = 6$. Model M9: (7) with five poles and two zeros, (8) numerical approach using $K = 1$, (9) numerical approach using $K = 2$. In all the partial models, the poles and zeros considered are the greater ones.

TABLE 3

Maximum values of K, used in the numerical filtering of a pole and depending on the s/n in the thermograms, to obtain maximum divergences of (a) 2 dB or (b) 10 dB in the transfer function of the models given in Table 1

	M8		M9		MI	
	a	b	a	b	a	b
40 dB	14	32	4	15	1	6
60 dB	6	14	2	6	1	2
80 dB	2	6	1	2	–	1

range 2–10 dB. An example, for a signal-to-noise ratio 60 dB, is shown in Fig. 1B.

Table 3 also includes the results corresponding to a partial intermediate model MI described by the four main poles and one zero in Table 1. This model is such that for values of the moduli of the transfer function 40, 60 and 80 dB, the corresponding frequencies are approximately the geometric mean between those of models M8 and M9.

In what concerns the analysis of the phase of the transfer function, Fig. 2A shows that the numerical filter does not introduce important modifications below the frequencies considered.

For the numerical integration (when filtering a zero) the optimum value of K to be used is always $K=1$. Greater values give rise to a progressive divergence in the modulus and, especially, in the phase of the filter, as shown in Fig. 2B.

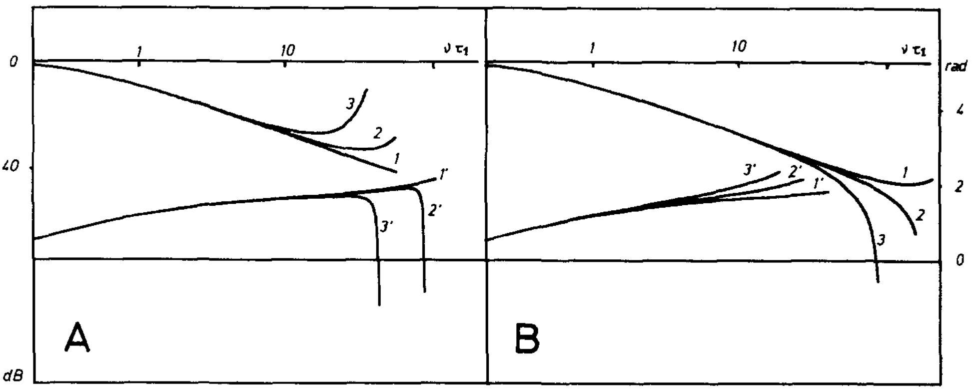

Fig. 2. Moduli in dB, vs. a relative frequency scale, of the transfer functions corresponding to a filter M9 with only the two main poles and the first zero. (A) Numerical approach of the filter, using $K=1$ for the zero and the following values for the poles: (1) $K=1$, (2) $K=4$, (3) $K=8$. (1′), (2′) and (3′) are the corresponding phases in rad. (B) Numerical approach of the filter, using $K=1$ for the poles and the following values for the zero: (1) $K=1$, (2) $K=4$, (3) $K=8$. (1′), (2′) and (3′) are the corresponding phases in rad.

CONCLUSIONS

For the different signal-to-noise ratios, those values of the parameters in the numerical algorithms which lead to optimum inverse filters have been obtained. The differences in the moduli of the transfer function between the exact filter and the numerical one are, when using these values, either less than 2 dB or less than 10 dB.

Standard numerical inverse filtering is an adequate deconvolution procedure for signal-to-noise ratios $s/n < 80$ dB. For larger ratios, however, a choice $\Delta t < \tau_1/300$ has to be considered.

Correct results are obtained (in the ranges of 2 or 10 dB, as specified in the text) in systems with s/n ranging from 40 to 60 dB, values usually found in actual experimental situations. For these systems, values of K between 1 and 4 have to be used, the choice depending on the presence of zeros in their transfer function.

For $s/n < 40$ dB it is no longer necessary to use $\Delta t \sim \tau_1/300$. Then, a value $\Delta t = \tau_1/60$ is adequate

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